Analysis of the Structure of Bulk Metallic Glasses Using EXAFS and EXELFS

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Beamline(s): **X23A2, X15B**

Introduction: There has been a rejuvenation of interest in the field of metallic glasses (BMGs) in the last decade, ever since the discovery of alloy compositions that allow the formation bulk glass[1, 2]. BMGs are defined as metallic glasses with minimum dimensions > 1mm [3]. We have chosen to examine the structure of the Pd-Ni-P system in order to explain, from an atomic structural point of view, its precipitously high glass-forming ability with respect to those of the binary alloys. EXAFS can provide information on the short-range order of glasses. The electron counterpart of EXAFS, the extended energy-loss fine structure (EXELFS), in addition, has higher spatial resolution to monitor fine structural changes. However, in the latter case, the analysis using K-edges becomes difficult for elements of high atomic number and one is restricted to the complicated but more accessible L edge, where the fine structure is a convolution of those from electrons of several L transitions.

Methods and Materials: One aspect of our research has been to develop the EXELFS of L-edges by doing comparative studies with K-edge EXAFS on fcc Ni and Cu. EXAFS data were collected at the X23A2 and X15B NSLS beamlines, and EXELFS data were collected at Lehigh University. The local structure around Pd, Ni and Cu in glassy Pd-Ni,Cu-P were then examined using EXAFS at the X23A2 NSLS beamline, while the P EXELFS was acquired at ONERA.

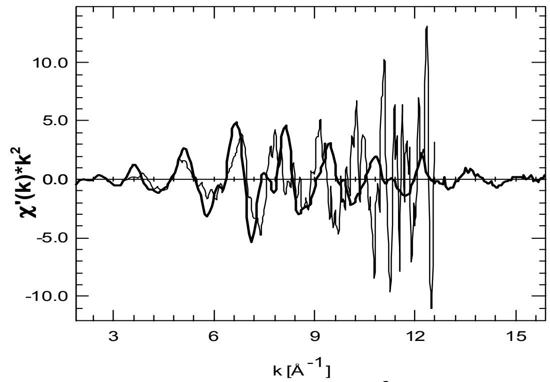

Figure 1. Comparison of the $\chi(k)*k^2$ function as obtained from L-edge EXELFS (thin line) with that obtained from K-edge EXAFS (thick line).

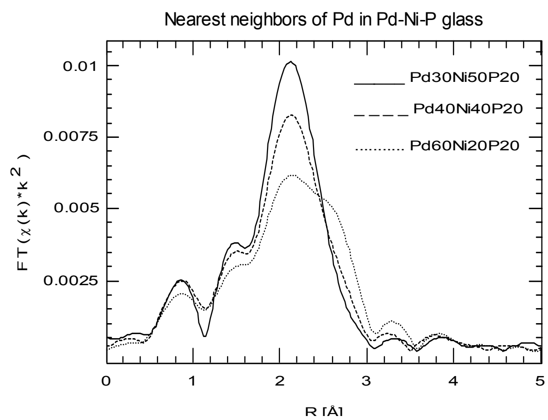

Figure 2. The partial radial distribution functions around Pd in the Pd-Ni-P system showing the two different structures at the ends of the Pd concentration and the mixed structure in between.

Results: Figure 1 shows the comparison between the $\chi(k)*k^2$ functions obtained from the EXELFS and EXAFS of the Ni L-edge and K-edge, respectively. As we can see, K-edge EXAFS, even with much poorer spatial resolution, provides a better signal to noise ratio and therefore a larger useful k-range for analysis. The manifestation of this in real-space is that the errors in coordination numbers are larger in L-edge EXELFS than in K-edge EXAFS[4].

We found two unique structures that mark the ends of bulk glass formation in this system, and at intermediate composition (where glass-stability is highest) the local structure was found to be a combination of these end compositions (Figure 2). A similar result was found from P EXELFS of these glasses. These findings agree well with XPS studies on the same glasses where it was found that the valence band structure of the $Pd_{40}Ni_{40}P_{20}$ glass was a linear combination of those of $Pd_{30}Ni_{50}P_{20}$ and $Pd_{60}Ni_{20}P_{20}$ glasses[5].

Conclusions: We can conclude from the comparative analysis that as a structural probe around high atomic number elements EXELFS provides is much poorer than EXAFS in terms experimental signal to noise ratio. Form our investigation of the Pd-Ni-P bulk metallic glass family, the alloy with the highest glass stability shows local structure from the two glasses that mark the ends of bulk glass formation.

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